Laboratory Name:Idaho National Laboratory
B&R Code: KC 0202010

FWP and possible subtask under FWP:
Structural and Electrostatic Effects in Self Assembled Nanostructure and Interface Growth.
FWP Number: 3E106 (100390)
Program Scope: This work includes two Tasks. The first is the research task designated in the title of this FWP, and the second is an administrative Task. Task 1; the goal of this work is to develop a fundamental understanding of how structural, electrostatic, and strain effects can be used to control the growth, morphology, magnetic, and electronic properties of interfaces and self-assembled nanostructures. The ability to control and direct the growth of interfaces and nanostructures on semiconductor surfaces is key to developing new electronic devices of importance for a variety of DOE missions, including national security. To this end, a variety of materials systems will be studied. While the primary focus will be on compound semiconductors with the zinc-blende structure, such as GaAs, elemental semiconductors, such as Si, will also be included. Extension of this work to new materials, including perovskites, will also be undertaken. Task 2; to provide assistance to the Solid State Physics and Materials Chemistry Branch, Division of Materials Science, Office of Basic Energy Science, of the Department of Energy. Technical assistance will be provided in reviewing programs and proposals, in formulating symposia and workshops, and performing special tasks.

Major Program Achievements (over duration of support):
Publications for 2005:

1.) Anion Effects at ZnSe/GaAs(100) Interfaces, H. H. Farrell and R. A. LaViolette., Vac. Sci. Technol. **B**. 23, 406 (2005)

2.) Semiempirical Inelelastic Mean Free Paths for Positrons, H. H. Farrell and A. B. Denison, Surface and Interface Analysis, 37, 529 (2005).

FY2005 marks several new changes in direction for this project. Upon the departure of R.A. LaViolette to SNL, The PI (Farrell) has assumed full responsibility for performing the first-principle calculations key to this work. As part of this process, she spent approximately a week at Accelrys being trained in the use of various calculational programs. In addition to ongoing work on equilibrium governed interfaces between III-V and II-VI compounds, this work has been expanded to include non-equilibrium compound formation. The materials currently under investigation include those with the generic formula $Mn_xGa_yAs_z$ and are of relevance to spintronic systems. More importantly, when completed these studies should offer insight into atomic motion in the presence of interface compound formation. A final change in direction for Task 1 involves the initiation of a new collaboration with Darrell Schlom and his research group at Pennsylvania State University on semiconductor-oxide interfaces.

For Task 2, several trips were made to Germantown, MD and SNL-W to support DMS/BES through reviewing proposals, selecting reviewers and performing other special tasks. Additional administrative support was provided from INL via electronic word processing.

Program impact:
The work performed under Task 1 is designed to increase our understanding of the forces that shape the detailed atomic nature of surfaces and interfaces under both equilibrium and non-equilibrium conditions.

Interactions:
University of Minnesota at Minneapolis (C. J. Palmstrom)
Pennsylvania State University (Darrell Schlom)

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask): Committee; Physics and Chemistry of Semiconductor Surfaces Annual Meetings.

Personnel Commitments for FY2005 to Nearest +/- 10%:
Helen H. Farrell, 75 %.

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA $220K FY04 BA $272K FY05 BA $ 265 K

Laboratory Name: Idaho National Enginering and Environmental Laboratory
B&R Code: KC 0202020

FWP and possible subtask under FWP:
High-Field Intermetallic Superconductors

FWP Number:
3E103 (100087)

Program Scope: The funding for this project was initially sent to INL to support Daniel Branagan's work on the magnetism CS&P project centered at BNL. When Branagan left INL, $ 41,024.18 remained of this funding. After consultation with G. A. Samara (SNL), Program Manager for the CS&P, these funds were transferred to Farrell and LaViolette to supplement the "High Field Intermetallic Superconductors" CS&P project, which was selected for FY2005. Following the demise of the CS&P program, this work became a stand alone project. The primary task undertaken was to use first-principles, density functional theory calculations to determine the thermodynamic stability, Fermi-level density of states and phonon spectra of potential intermetallic superconductors containing off-stoichiometry transition metal diborides. It should be noted that LaViolette moved to SNL near the end of February, 2005.

Major Program Achievements (over duration of support):
Using first-principles, density functional theory calculations, we have shown that the increase in superconducting critical temperature to above 9 K experimentally observed for B-rich, off-stoichiometry NbB_2 material is associated with the formation of B dimers on Nb sites rather than with the formation of Nb vacancies, as previously proposed. Our calculations show that certain of these B dimer configurations have lower binding energies than do the vacancy structures. This result is pressure independent in the range between 0 and 10 GPa, and above. Further, the dimer-containing materials have a higher electronic density of states at the Fermi level than do the vacancy structures. Finally, the presence of B dimers results in the splitting off of phonon normal modes. These last two factors are relevant to the improved superconducting properties. This work has been written up as a paper entitled "Diatomic Substitutionals in Superconducting $Nb_{(1-x)}B_2$" by H. H. Farrell, R. A. LaViolette and T. M. Lillo, and is being submitted to Physica C.

Program impact:
This work provides insight into superconductivity in the MgB_2 family of materials. It suggests new lines of enquiry for both MgB_2 itself (e.g., the formation of carbon dimers) and for other P6/mmm compounds. Finally, it provided the "experimental" results that inspired a separate, LDRD funded, project that has led to a simplification of the McMillan formalism for predicting critical temperatures for compounds having an Einstein frequency distribution of phonon modes involved in the electron-phonon interaction governing T_c.

Interactions:
R. A. LaViolette (SNL).

Recognitions, Honors and Awards (at least partly attributable to support under this FWP or subtask):
None.

Personnel Commitments for FY2005 to Nearest +/- 10%:
15 %

Authorized Budget (BA) for FY03, FY04, FY05:
FY03 BA $ 0 K **FY04 BA $** 0 K **FY05 BA** $ 41 K